

Canadian Journal of Chemistry

Contents
Volume 74, 1996

Revue canadienne de chimie

Sommaire
Volume 74, 1996

January / Janvier

REVIEW / SYNTHÈSE

Annette Bernas, Christiane Ferradini et Jean-Paul Jay-Gerin Électrons en excès dans les milieux polaires homogènes et hétérogènes 1

ARTICLES

Karen Bell, Endang Saepudin, and Paul Harrison Irreversible inhibition of 3-hydroxy-3-methylglutaryl-coenzyme A synthase from yeast by F-244 and (*RS*)- β -butyrolactone 24

Carole Savoie and Christian Reber Near-infrared and visible luminescence and absorption spectroscopy of low-coordinate organometallic rhenium compounds 28

Christopher Owen Bender Mechanistic variations in the formation of benzocyclooctatetraene from benzobicyclo[4.2.0]octa-2,4,7-triene 32

Chui Har Leon-Lai, Michael J. Gresser, and Alan S. Tracey Influence of vanadium(V) complexes on the catalytic activity of ribonuclease A. The role of vanadate complexes as transition state analogues to reactions at phosphate 38

Marta Luiz, Arnaldo T. Soltermann, Alicia Biasutti, and Norman A. García A kinetic study on singlet molecular oxygen ($O_2(^1\Delta_g)$) generation and quenching by dihydroxynaphthalenes 49

J.C. Gard, B. Hanquet, L. Roullier, Y. Mugnier, and J. Lessard Electrochemically induced chain reactions: the addition of fluorene and indene to aromatic aldehydes initiated by electrochemical reduction 55

V. Jayalakshmi and R. Ramaswamy Novel experimental findings in the B-Z system employing mixed substrates 64

Zbigniew Zimpel, Barbara R. Nelson, and John A. Weil SCF-MO computational analysis of the geometric conformation and charge distribution in picric acid and alkali picrate salts 70

T.S. Sorensen and F. Sun *In situ* preparation of cyclopropanones with the bicyclo[3.1.0]hexan-6-one skeleton (substituted examples of the Loftfield intermediate). Confirmation of a very facile intramolecular alkyl cyclopropanone-dienol rearrangement 79

Don M. Coltart and James L. Charlton The asymmetric synthesis of aryltetralin lignans: (–)-isolariciresinol dimethyl ether and (–)-deoxysikkimotoin 88

A. Safavi and M.B. Gholivand Electrochemical investigation of reduction of mercury complexes of 2-aminocyclopentene-1-dithiocarboxylic acid and some of its derivatives at mercury electrodes 95

Luis García Rodenas, Mauricio Chocrón, Pedro J. Morando, and Miguel A. Blesa Radiation-induced dissolution of chromium oxide in aqueous solutions 103

Valerie J. Jefford, Melbourne J. Schriver, and Michael J. Zaworotko The selective complexation of adamantane nitriles by tungsten pentacarbonyl 107

Branko S. Jursic AM1 semiempirical study of benzopyrroles as dienes for Diels-Alder reaction 114

Begoña García, Francisco J. Hoyuelos, Rafael Alcalde, and José M. Leal Molar excess volumes of binary liquid mixtures: 2-pyrrolidinone with C_6 - C_{10} *n*-alkanols 121

Notice to authors / Note aux auteurs IFC

Editorial / Éditorial iii

IUPAC recommendations / Recommandations de l'UICPA v

Author Index / Index des auteurs AI-1

Instructions to authors / Recommandations aux auteurs I-1

NRC Research Press Publication Policy / Presses scientifiques du CNRC, politique de publication vii

February / Février

ARTICLES

Pascal Langlois, Pierre Soucy, Yves L. Dory, and Pierre Deslongchamps Transannular Diels-Alder cyclization of substituted 13-membered trienes. An approach to the B.C.D.[6.6.5] rings of the 14 β -hydroxysteroids 129

Fernande D. Rochon, Robert Melanson, Eryk Thouin, André L. Beauchamp, and Corinne Bensimon	Synthesis and study of Pt(II)-nitrile complexes. Multinuclear NMR spectra and crystal structures of compounds of the types $[\text{Pt}(\text{R-CN})\text{Cl}_3]^-$ and <i>cis</i> and <i>trans</i> - $\text{Pt}(\text{R-CN})_2\text{Cl}_2$	144
Lorraine Couture, Jacques E. Desnoyers, and G��rald Perron	Some thermodynamic and transport properties of lithium salts in mixed aprotic solvents and the effect of water on such properties	153
Youla S. Tsantrizos, Sotiria Pischos, Fran��oise Sauriol, and Paul Widden	Peptaibol metabolites of <i>Tolypocladium geodes</i>	165
Theodore M. Garver, Karen Joy Maa, and Kirk Marat	Conformational analysis and 2D NMR assignment strategies for lignin model compounds. The structure of acetoguaiacyl-dehydro-diisoeugenol methyl ether	173
T.A. Keith and R.F.W. Bader	Properties of atoms in molecules: nuclear magnetic shielding	185
Pradip K. Bakshi, T. Stanley Cameron, and Osvald Knop	Crystal chemistry of tetradial species. Part 8. Mix and match: cation geometry, ion packing, hydrogen bonding, and π - π interactions in <i>cis</i> -2,2'-bipyridinium(1+) and 1,10-phenanthroline(1+) tetraphenylborates — and what about proton sponges?	201
Richard Connors, Elisabeth Tran, and Tony Durst	Acyl cyanides as carbonyl heterodienophiles: application to the synthesis of naphthols, isoquinolones, and isocoumarins	221
Tsukasa Iwadare, Yoshiyuki Ichinohe, and Kazuhiko Orito	Decomposition of tosylhydrazones of benzoin, benzoin acetate, and benzoin benzoate with alkali and metal complex hydrides	227
J. Bouchard, C. Maine, R.M. Berry, and D.S. Argyropoulos	Kraft pulp bleaching using dimethyldioxirane: stability of the oxidants	232
J. Balsevich, G. Bishop, S.L. Jacques, L.R. Hogge, D.J.H. Olson, and N. Lagani��re	Preparation and analysis of some acetosugar esters of abscisic acid and derivatives	238
Ian M. Walker and Paul J. McCarthy	Single-crystal polarized spectra in the near-infrared region: a local-mode analysis of the spectra of $\text{M}_2\text{MnCl}_4 \cdot 2\text{X}_2\text{O}$ (M = Cs, Rb; X = H, D)	246
Jason V. Jollimore, Marc Vacheresse, Keith Vaughan, and Donald L. Hooper	The effect of <i>ortho</i> and <i>para</i> substituents on the formation of the <i>E</i> and <i>Z</i> isomers of the arylhydrazones obtained from diazonium coupling with methyl 3-aminocrotonate and 3-aminocrotononitrile	254
William J. Leigh, T. Johnathan Lewis, Vincent Lin, and J. Alberto Postigo	The photochemistry of 3,3',4,4'-tetramethoxy- and 4-hydroxy-3,3',4'-trimethoxystilbene — models for stilbene chromophores in peroxide-bleached, high-yield wood pulps	263
Author Index / Index des auteurs		AI-1

March / Mars

ARTICLES

Alain Berthod, Jun Xiang, Serge Alex et Colette Gonnet-Collet	Chromatographie �� contre courant et micelles inverses pour la s��paration et l'extraction de cations m��talliques	277
Antonio Lorente, Marta Casillas, Pilar Gomez-Sal, and Antonio Manzanero	2-Azabuta-1,3-diene-4-carbonitriles: stereoselective synthesis and nucleophilic substitution at the carbon-nitrogen double bond	287
F. Rey, M.A. Ferreira, P. Facal, and A.A.S.C. Machado	Effect of concentration, pH, and ionic strength on the viscosity of solutions of a soil fulvic acid	295
Yixing Zhao and Gordon R. Freeman	Solvent effects on the reactivity of solvated electrons with organic solutes in 1-butylamine-water mixtures	300
Clifford C. Leznoff and David M. Drew	The use of bisphthalonitriles in the synthesis of side-strapped 1,11,15,25-tetrasubstituted phthalocyanines	307
Raymond U. Lemieux, Ulrike Spohr, Mimi Bach, Dale R. Cameron, Torben P. Frandsen, Bjarne B. Stoffer, Birte Svensson, and Monica M. Palcic	Chemical mapping of the active site of the glucoamylase of <i>Aspergillus niger</i>	319
Acharee Tiyyabhorn and K. Omar Zahir	Quantum yield of singlet dioxygen and elucidation of the quenching mechanism for the reaction between the doublet excited states of tris(bipyridine)chromium(III) and triplet dioxygen	336
Witold Neugebauer, Eric Pinet, Munsok Kim, and Paul R. Carey	Modified method of synthesis of N-substituted dithioesters of amino acids and peptides in the Pinner reaction	341
Hongbo Su and Michael Thompson	Rheological and interfacial properties of nucleic acid films studied by thickness - shear mode sensor and network analysis	344
Jos�� Luis Lucas Vaz, G��rard Duc, Michelle Petit-Ramel, Ren�� Faure, and Olivier Vittori	Cd(II) complexes with phthalic acid: solution study and crystal structure of cadmium(II) phthalate hydrate	359
Maria P. Ros, Jesus Thomas, Guillermo Crovetto, and Juan Ll��r	Kinetics and mechanism of covalent addition of S(IV) species to the acridinium cation	365
Romano Andrade, William A. Ayer, and Latchezar S. Trifonov	The metabolites of <i>Trichoderma longibrachiatum</i> . Part II. The structures of trichodermolide and sorbiquinol	371
Behzad Mahdavi, Danielle Miousse, Jo��l Fournier, Hugues M��nard, and Jean Lessard	Hydrogen evolution reaction at nickel boride electrodes in aqueous and in aqueous methanolic and ethanolic solutions	380

Yunjun Wang, Paul G. Scott, Jan Sejbál, and George Kotovych Evidence for the role of the α -helix in the xylosylation reactions involving the glycosaminoglycan-bearing serine of decorin/DS-PGII as shown by ^1H NMR, CD, and molecular modeling studies	389
James Malcolm Sangster Calculation of phase diagrams and thermodynamic properties of 18 binary common-ion systems of Na,K,Ba/F,F,MoO ₄ ,WO ₄	402
George M. Strunz and Heather J. Finlay Expedient synthesis of unsaturated amide alkaloids from <i>Piper</i> spp: Exploring the scope of recent methodology	419
Long Mao, Steven J. Rettig, Robert C. Thompson, James Trotter, and Shihua Xia 2,3-Pyrazinedicarboxylates of cobalt(II), nickel(II), and copper(II); magnetic properties and crystal structures	433
Wolfgang Kliegel, Ute Schumacher, Steven J. Rettig, and James Trotter Structural studies of organoboron compounds LXIV. Boron chelate formation with glycolhydroxamic acids, and the crystal and molecular structure of 5-(1-hydroxycyclohexyl)-2,2-diphenyl-1,3-dioxo-4-azonia-2-borata-4-cyclopentane	445
COMMUNICATION	
Peter Buist, Dale Marecak, Brian Dawson, and Bruce Black Use of ^{19}F NMR as a direct probe of Δ^9 desaturase cryptoregiochemistry: a feasibility study	453
Author Index / Index des auteurs	AI-1

April / Avril

ARTICLES

Annette D. Allen, Jim D. Colomvakos, Ian Egle, Ronghua Liu, Jihai Ma, Romeo M. Marra, Michael A. McAllister, and Thomas T. Tidwell 1995 R.U. Lemieux Award Lecture: Ketenes and bisketenes: organic chemistry in microcosm	457
Peter Wan, Beverly Barker, Li Diao, Maike Fischer, Yijian Shi, and Cheng Yang 1995 Merck Frosst Award Lecture: Quinone methides: relevant intermediates in organic chemistry	465
Jailson Farias de Lima and Neyde Yukie Murakami Iha Wavelength dependence and solvent effects on the ligand field photochemistry: the ring closure process in the excited $[\text{Fe}(\text{CN})_5(\text{tn})]^{3-}$ complex	476
Olivier Gaud, Robert Granet, Mourad Kaoudji, Pierre Krausz, Jean Claude Blais et Gerard Bolbach Synthèse et analyse structurale de nouvelles méso-arylporphyrines glycosylées en vue de l'application en photothérapie des cancers	481
Raphaël Sabbah et Meriem Gouali Énergétique des liaisons inter et intramoléculaires dans les trois isomères de l'aminophénol	500
Svetlana V. Kudrevich, Maria G. Galpern, Evgeny A. Luk'yanets, and Johan E. van Lier Substituted tetra-2,3-pyrazinoporphyrazines. Part I. Angular annelation of tetra-2,3-quinoxalinoporphyrazine	508
P. Caravan, Suzanne M. Budge, and John M. Roscoe The reactions of $\text{O}(\text{C}^2\text{P})$ with some carboxylic acids and esters	516
N.H. Werstiuk, R.S. Brown, and Q. Wang An AM1 calculational study of the protonation and reactions of 3,4-dihydro-2-oxo-1,4-ethanoquinoline, 3,4-dihydro-2-oxo-1,4-propanoquinoline, 3,3,4,5-tetrahydro-2-oxo-1,5-ethanobenzazepine, 3,3,4,5-tetrahydro-2-oxo-1,5-propanobenzazepine, and <i>N</i> -methyl-4-bromo-2-methylacetanilide	524
Ivan Cordova-Reyes, Hanbin Hu, Jian-Hua Gu, Elizabeth VandenHoven, Ali Mohammed, Steven Holdcroft, and B. Mario Pinto Synthesis and characterization of polymer-bound selenium coronands: enhancing the stability of reactive dications by restricting intermolecular interactions	533
Dennis Suh, David L. Pole, John Warkentin, and Johan K. Terlouw Intramolecular 1,2-alkyl shifts in unsymmetric dialkoxycarbenes studied by very low vapour pressure (VLVP) pyrolysis – mass spectrometry	544
Pradip K. Bakshi, Margaret A. James, T. Stanley Cameron, and Osvald Knop Polyhalide anions in crystals. Part I. Triiodides of the Me_4N^+ , Me_4P^+ , quinuclidinium, 1-azoniapropellane, and 1,4-diazoniabicyclo[2.2.2]octane (DabcoH_2^{2+}) cations, and 1,10-phenanthroline(1+) tribromide	559
H. Alarabi, R.A. Bell, H.E. Howard-Lock, J. Kowanetz, and C.J.L. Lock <i>N</i> 10-(2'-Mercaptoethanoyl)-2,2,5,5-tetramethyl-3,4-dithia-7,10-diazabicyclo[5.3.0]decane and its reaction with oxotrichlorobis(triphenylphosphine)rhenium(V)	574
Kingsley K. Donkor, Byron Kratochvil, and M. John M. Duke Estimation of the fines content of Athabasca oil sands using instrumental neutron activation analysis	583
George R. Elia, Ronald F. Childs, James F. Britten, Daniel S.C. Yang, and Bernard D. Santarsiero Structure and wavelength modification in retinylidene iminium salts	591
Donald R. Arnold, Dennis A. Connor, Kimberly A. McManus, Pradip K. Bakshi, and T. Stanley Cameron The photochemical nucleophile-olefin combination, aromatic substitution (photo-NOCAS) reaction. Part I: Involving (<i>R</i>)-(+)- α -terpineol and (<i>R</i>)-(+)-limonene, substituting on 1,4-dicyanobenzene	602
Jean-Claude Hallé, Jacques Lelievre, and François Terrier Solvent effect on preferred protonation sites in nicotinate and isonicotinate anions	613
Stephen Hanessian and Jean-Yves Sanceau Asymmetric synthesis of taxol and taxotère side chains by enolate hydroxylation	621
Neeta Jalani, Seema Kothari, and Kalyan K. Banerji Correlation analysis of reactivity in the addition of substituted benzylamines to β -nitrostyrene	625
Author Index / Index des auteurs	AI-1

May / Mai

ARTICLES

Thomas W. Swaddle Reflections on the outer-sphere mechanism of electron transfer	631
Loren G. Hepler and Jamey K. Hovey Standard state heat capacities of aqueous electrolytes and some related undissociated species	639
Alaa S. Abd-El-Aziz, Christine R. de Denus, Karen M. Epp, Simone Smith, Richard J. Jaeger, and David T. Pierce Effect of ligand structure, solvent, and temperature on the electrochemical behavior of polyarene-iron complexes	650
Kefei Wang and R.B. Jordan Electron transfer kinetics of cobaloxime complexes	658
James P. Kutney, Yong-Huang Chen, and Steven J. Rettig The chemistry of thujone. XVIII. Homothujone and its derivatives	666
Reno F. DeBono, Glenn D. Loucks, Deborah Della Manna, and Ulrich J. Krull Self-assembly of short and long-chain <i>n</i> -alkyl thiols onto gold surfaces: A real-time study using surface plasmon resonance techniques	677
Philippe Brunet and James D. Wuest Formal transfers of hydride from carbon-hydrogen bonds. Attempted generation of H ₂ by intramolecular protonolyses of the activated carbon-hydrogen bonds of dihydrobenzimidazoles	689
Mourad Elhabiri, Paulo Figueiredo, Florian George, Jean-Paul Cornard, André Fougerousse, Jean-Claude Merlin, and Raymond Brouillard Ground- and excited-state properties of some naphthoflavilyums	697
William E. Lee and H. Gail Thompson Detection of Newcastle disease virus using an evanescent wave immuno-based biosensor	707
Steven Hiroshi Tanaka, Hikari Infinity Yoshihara, Alice Wen-Chi Ho, Frankie W. Lau, Peter Westh, and Yoshikata Koga Excess partial molar enthalpies of alkane-mono-ols in aqueous solutions	713
Hongyan Luo and Chris Orvig Rhodium complexes of <i>P,P',P''</i> -tetrakis(<i>o</i> -hydroxyphenyl)diphosphinoethane	722
Chao-Mei Yu, Jonathan M. Curtis, Jeffrey L.C. Wright, Stephen W. Ayer, and Ziba R. Fathi-Afshar An unusual fatty acid and its glyceride from the marine fungus <i>Microsphaeropsis olivacea</i>	730
Oswald S. Tee, Timothy A. Gadosy, and Javier B. Giorgi Dissociation constants of host-guest complexes of alkyl-bearing compounds with β -cyclodextrin and "hydroxypropyl- β -cyclodextrin"	736
Timothy A. Gadosy and Oswald S. Tee Spectator catalysis in the cleavage of <i>p</i> -nitrophenyl acetate and <i>p</i> -nitrophenyl hexanoate by "hydroxypropyl- β -cyclodextrin"	745
Shermin Rahim and John Milne Studies on the interaction of selenite and selenium with sulphur donors. Part 4. Thiosulfate	753
Sekh Mahiuddin Mixed alkali effect in sodium thiocyanate - potassium thiocyanate - acetamide melt systems	760
Wei Xu, Jagadeese J. Vittal, and Richard J. Puddephatt Propargyl calix[4]arenes and their complexes with silver(I) and gold(I)	766
Author Index / Index des auteurs	AI-1

June / Juin

This issue is dedicated to Professor Richard F.W. Bader
Ce tirage est dédié au Professeur Richard F.W. Bader

ARTICLES

Toshikatsu Koga, Hidenori Aoki, and Ajit J. Thakkar Kinetic energy analysis of atomic multiplets. II. $s^m d^n$ configurations	775
David M. Bishop Dispersion formulas for real- and imaginary-frequency-dependent hyperpolarizabilities	781
Jaime M. Martell, James B. Tee, and Russell J. Boyd Topological properties of the electronic structures of the reactants, transition states, and products of the reactions of the hydroxyl radical with the series $C_2H_nF_{6-n}$, $n = 1-6$	786
Ralf Stegmann and Gernot Frenking Analysis of magnesium-carbon bonding in magnesium anthracene systems	801
William M. Davis and John D. Goddard The 1,2,3,5-ditelluradiazolyl $[HCN_2Te_2]$ species. Theoretical characterizations of the cation, radical, and radical dimers	810
Alex D. Bain and G.J. Duns A unified approach to dynamic NMR based on a physical interpretation of the transition probability	819
O. Novaro Non-additivity of intermolecular forces in helium and beryllium clusters	825
Paul L.A. Popelier On the differential geometry of interatomic surfaces	829
Steven M. Bachrach and Laureta M. Perriott Theoretical examination of the Diels-Alder reaction of 1,3-butadiene with cyclopentadiene and 2 <i>H</i> -phosphole	839
Cássia C. Turci, Stephen G. Urquhart, and Adam P. Hitchcock Inner-shell excitation spectroscopy of aniline, nitrobenzene, and nitroanilines	851
Yoram Tal Cohesive properties of metals as determined from atomic charge densities	870
Nick Henry Werstiuk and Jiangong Ma Applications and evaluation of IGAIM ¹³ C and ¹ H chemical shift calculations for unsaturated hydrocarbons and organolithium compounds	875
Hanno Essén and Arne Nordmark Some results on the electrostatic energy of ionic crystals	885

Kenneth B. Wiberg, Paul von Rague Schleyer, and Andrew Streitwieser	The role of hydrogens in stabilizing organic ions	892
O. Mó and M. Yáñez	The theory of atoms in molecules as a tool to investigate the reactivity of tetraphosphacubane	901
Zhi-Xiang Wang, Ruo-Zhuang Liu, Ming-Bao Huang, and Zhonghua Yu	An ab initio study on the insertion reactions of CH ($X^2\Pi$) with NH_3 , H_2O , and HF	910
Josef Paldus and Xiangzhu Li	Calculation of static molecular properties in the framework of the unitary group based coupled cluster approach	918
Clinton D. Bryan, K. Barbara Schowen, and Richard L. Schowen	Solvent isotope effects as a probe of general catalysis and solvation in phosphoryl transfer	931
I. Mayer	Orthogonal effective atomic orbitals in the topological theory of atoms	939
C.G. van Beek, J. Overeem, J.R. Ruble, and B.M. Craven	Electrostatic properties of ammonium fluoride and deuterated ice- I_h	943
William J. Leigh, J. Alberto Postigo, and K.C. Zheng	Cyclobutene photochemistry. Adiabatic photochemical ring opening of alkylcyclobutenes	951
Dennis P. Clougherty	On the stability of endohedral rare gas fullerenes	965
N.H. March	Local energy and chemical potential equations and the exchange-correlation potential	969
Christof Hättig, Georg Jansen, Bernd A. Heß, and János G. Ángyán	Topologically partitioned dynamic polarizabilities using the theory of atoms in molecules	976
Andre D. Bandrauk, Hengtai Yu, and Eric E. Aubanel	Coherent control of electrons in molecules	988
Axel D. Becke	Current-density dependent exchange-correlation functionals	995
Pablo J. Bruna and James S. Wright	Strongly bound doubly excited states of Be_2	998
Delano P. Chong	Density-functional calculation of core-electron binding energies of glycine conformers	1005
Geoffrey Hunter	Atoms in molecules from the exact one-electron wave function	1008
Yosslen Aray and Jesús Rodríguez	Study of NO and CO dissociation on the (100) Cu surface using density functional theory and the topological analysis of the electronic density and its Laplacian	1014
Krisztina L. Malisza, Lijuan Li, and Michael J. McGlinchey	Delocalized bonding in tetrahedral organo-transition metal clusters: an EHMO study of metal vertex rotations in $Co_2Fe(CO)_9S$, $CpMoCo_2(CO)_8CR$, and in $Cp_2Mo_2(CO)_4(RC\equiv CR)$	1021
Xabier Lopez, Jesus M. Ugalde, Cecilia Sarasola, and Fernando P. Cossio	On the accuracy of density functional theory for ion-molecule clusters. A case study of PL_n^+ clusters of the first and second row hydrides	1032
Juergen Hinze, F. Biegler-König, and A.G. Lowe	Molecular charge density analysis	1049
R.Y. de Vries, W.J. Briels, D. Feil, G. te Velde, and E.J. Baerends	Charge density study with the Maximum Entropy Method on model data of silicon. A search for non-nuclear attractors	1054
Ian Bytheway, Paul L.A. Popelier, and Ronald J. Gillespie	Topological studies of the charge density of some group 2 metallocenes $M(\eta^5-C_5H_5)_2$ ($M = Mg$ or Ca)	1059
V. Sreedhara Rao, Amrendra Vijay, and A.K. Chandra	A comparative study of the energetics, structures, and mechanisms of the $HCN \leftrightarrow HNC$ and $LiCN \leftrightarrow LiNC$ isomerizations	1072
Paul J.A. Ruttink, Peter C. Burgers, and Johan K. Terlouw	Proton and electron transfers in O-H-O and C-H-O hydrogen-bridged ions: their role in the dissociation chemistry of ionized acetol, $CH_3C(=O)CH_2OH^+$	1078
A. Savin, B. Silvi, and F. Colonna	Topological analysis of the electron localization function applied to delocalized bonds	1088
E.V. Ludeña, R. López-Boada, and R. Pino	Approximate kinetic energy density functionals generated by local-scaling transformations	1097
Akitomo Tachibana	Zero-temperature equation-of-motion of electron pair in the BCS theory of superconductivity	1106
Félix Rosillo, Yosslen Aray, Jesús Rodríguez, and Juan Murgich	The topology of the valence shell and the electric field gradient at the nitrogen nucleus in aziridines	1116
Roman F. Nalewajski, Janusz Mrozek, and Grzegorz Mazur	Quantum chemical valence indices from the one-determinantal difference approach	1121
Keith E. Laidig	Atomic origins of molecular polarizabilities	1131
Kathleen M. Gough, Margaret M. Yacowar, Richard H. Cleve, and Jason R. Dwyer	Analysis of molecular polarizabilities and polarizability derivatives in H_2 , N_2 , F_2 , CO , and HF , with the theory of atoms in molecules	1139
Pietro Roversi, Mario Barzaghi, Felicita Merati, and Riccardo Destro	Charge density in crystalline citrinin from X-ray diffraction at 19 K	1145
Ting-Hua Tang and Yun-Ping Cui	A theoretical study of some $X-H \cdots \pi$ hydrogen-bonded complexes using the theory of atoms in molecules	1162
Vladimir G. Tsirelson	Topological analysis of the experimental electron density	1171
Sean A.C. McDowell, Ashok Kumar, and William J. Meath	Anisotropic and isotropic triple-dipole dispersion energy coefficients for all three-body interactions involving He, Ne, Ar, Kr, Xe, H_2 , N_2 , and CO	1180
Jiahu Wang, B. James Clark, Hartmut Schmider, and Vedene H. Smith, Jr.	Topological analysis of electron momentum densities and the bond directional principle: the first-row hydrides, AH , and homonuclear diatomic molecules, A_2	1187

D.A. Armstrong, D. Yu, and A. Rauk Oxidative damage to the glycyl α -carbon site in proteins: an ab initio study of the C—H bond dissociation energy and the reduction potential of the C-centered radical	1192
Rainer Glaser and Christopher J. Horan Interpretation of neighboring group interactions in crystal structures. A solid state and quantum-chemical study of "incipient nucleophilic attack" in 2-diazonium benzoic acid and its benzoate	1200
Keith E. Laidig, Peter Speers, and Andrew Streitwieser Origin of depressed dipole moments in five-membered, unsaturated heterocycles	1215
Camilla Scott and Friedrich Grein The anomeric effect in first-row/second-row acetal-like systems	1221
Mark Eberhart From topology to geometry	1229
T.-T. Nguyen-Dang, F. Châteauneuf, and S. Manoli Molecules in high-intensity laser fields	1236
Dietmar Krause and Mariusz Klobukowski On the performance of molecular model core potential orbitals in spin-orbit and electron correlation studies	1248
Jordi Mestres, Miquel Duran, and Juan Bertrán Comparative electronic analysis between hydrogen transfers in the $\text{CH}_4/\text{CH}_3^+$, $\text{CH}_4/\text{CH}_3^-$, and $\text{CH}_4/\text{CH}_3^\cdot$ systems: on the electronic nature of the hydrogen (H^- , H^\cdot , and H^+) being transferred	1253
Boris B. Stefanov and Jerzy Cioslowski Variability of shapes and properties of atoms in molecules: a case study of the carbonyl oxygen	1263
Curt M. Breneman and Lawrence W. Weber Charge and energy redistribution in sulfonamides undergoing conformational changes. Hybridization as a controlling influence over conformer stability	1271
Author Index / Index des auteurs	AI-1

July / Juillet

ARTICLES

J. Peter Guthrie 1995 Syntex Award Lecture: Correlation and prediction of rate constants for organic reactions	1283
Tadeusz Górecki, Anna Boyd-Boland, Zhouyao Zhang, and Janusz Pawliszyn 1995 McBryde Medal Award Lecture: Solid phase microextraction — a unique tool for chemical measurements	1297
Melvin J. Farquharson and J. Stephen Hartman Bis(pyridine)difluoroboron, tris(pyridine)fluoroboron, and other (pyridine)haloboron cations. A systematic NMR study	1309
James C. Fishbein and Robert A. McClelland Halide ion trapping of nitrenium ions formed in the Bamberger rearrangement of <i>N</i> -arylhydroxylamines. Lifetime of the parent phenylnitrenium ion in water	1321
Jennifer L. Mueller, Martin S. Gibson, and J. Stephen Hartman Carbon-13 chemical shifts of alkene carbons in 2-acylidene-3,5-diaryl-2,3-dihydro-1,3,4-thiadiazoles and related benzothiazoles and -selenazoles, and their relationship to other push-pull alkenes	1329
David L. Pole, Pradeep K. Sharma, and John Warkentin Methoxy-(2-trimethylsilyl)ethoxycarbene. Reactions with Michael acceptors, with hydroxylic compounds, and with miscellaneous functional groups	1335
Jean-Jacques Bosc, Christian Jarry, Jamal Ouhabi, Michel Laguerre, and Alain Carpy New investigation of the reaction of 2-amino-2-oxazolines with isocyanates and isothiocyanates. Evidence of a transposition during the second step	1341
Paolo Strazzolini, Angelo G. Giumanini, Alberto Gambi, Giancarlo Verardo, and Giovanni Cerioni Preparation, spectroscopic properties, and ion chemistry of 3-diazo-1,1,1-trifluoro-2-propanone	1348
Kun H. Chung, Seog W. Rhee, Hyun S. Shin, and Christopher H. Moon Probe of cadmium(II) binding on soil fulvic acid investigated by ^{113}Cd NMR spectroscopy	1360
I. Egle, V. Gabelica, A.J. Kresge, and T.T. Tidwell The acid-catalyzed demetalation of 1-(tri- <i>n</i> -butylstannyl)-2-phenylethyne. A surprisingly small β -stannyl effect	1366
E.A. Jefferson, A.J. Kresge, and S.W. Paine Acid-catalyzed hydrolysis of 4-diazo-3-isochromanone: the effect of coplanarity on the carbon protonation of α -phenyl- α -carbonyldiazo compounds	1369
A.J. Kresge and S.W. Paine Carbon protonation of some phenylnamines in concentrated aqueous perchloric acid solution. Lowering of the upper limit for the $\text{p}K_a$ of phenylnammonium ions	1373
Stephen J. Loeb and James R. Mansfield Platinum(II) complexes of the tridentate thioether ligands $\text{RS}(\text{CH}_2)_3\text{S}(\text{CH}_2)_3\text{SR}$ ($\text{R} = \text{Et}, \text{iPr}, \text{Ph}$). Structures of $[\text{PtCl}(\text{iPrS}(\text{CH}_2)_3\text{S}(\text{CH}_2)_3\text{SiPr})][\text{BF}_4]$, $[\text{Pt}(\text{PhS}(\text{CH}_2)_3\text{S}(\text{CH}_2)_2\text{SPh})][\text{BF}_4]$, and $[\text{Pt}(\text{PPh}_3)(\text{iPrS}(\text{CH}_2)_3\text{S}(\text{CH}_2)_3\text{SiPr})][\text{BF}_4]_2 \cdot \text{CH}_2\text{Cl}_2$	1377
Yves Simon, Gérard Scacchi et François Baronnet Études des réactions d'oxydation du <i>n</i> -heptane et de l'isooctane	1391
David H. Jones and A. Scott Hinman Determination of the visible spectra of electrode reaction products in strongly absorbing media by diffusion-controlled chronoabsorptometry	1403
Anne-Marie Martre, Guy Mousset, Veronica Cosoveanu et Virginia Danciu Électroréduction de dérivés dinitrés aromatiques. V. Influences du matériau d'électrode et de systèmes rédox sur les réductions du 4,4'-dinitrodibenzyle et de l'acide 4,4'-dinitrostilbène-2,2'-disulfonique	1409
Dale E. Ward, Thomas E. Nixey, Yuanzhu Gai, Matthew J. Hrapchak, and M. Saeed Abaee Intramolecular Diels-Alder reactions of 2 <i>H</i> -thiopyran dienes	1418
Author Index / Index des auteurs	AI-1

August / Août

ARTICLES

- G.W. Buchanan, A. Moghimi, and C.I. Ratcliffe** Molecular motion in crown ethers. Application of ^{13}C and ^2H NMR to the study of 4-carboxybenzo-24-crown-8 ether and its KNCS complex in solution and in the solid phase 1437
- David Budac and Peter Wan** Excited state carbon acid dissociation and competing photorearrangements of 5*H*-dibenzo[*a,c*]cycloheptene derivatives 1447
- Andrzej Wawer and Jerzy Szydłowski** Hydrogen isotope fractionation between methanol and diphenylphosphine or dimethylphosphine in the gas phase and in aprotic solvents 1465
- Christopher Roos, Graham A. McGibbon, and Michael A. Brook** The thermolysis of ε -halodisilanes: a preference for 1,2-Si Si \rightarrow O rearrangement or Si—O cleavage over Si=O bond formation 1470
- Hui-Teng Er, David L. Pole, and John Warkentin** (Alkylthio)- and (phenylthio)methoxycarbenes from oxadiazolines 1480
- Margaret Ann James, Jason A.C. Clyburne, Anthony Linden, Bruce D. James, John Liesegang, and Vilma Zuzich** Structural diversity in thallium chemistry: structures of four chlorothallate(III) salts including a novel compound containing three geometrically different anions 1490
- Russell A. Bell, Donald W. Hughes, Colin J.L. Lock, and John F. Valliant** The synthesis and high-resolution NMR spectroscopy of ethyl *N*-(2-triphenylmethylthio)ethanoyl-*O*-(4'-[4''-(1''-bis(2'''-chloroethyl)amino)phenyl]butanoyl)-*L*-seryl-*S*-benzyl-*L*-cysteine: a chelate-chlorambucil complex for use as a ligand for $^{99\text{m}}\text{Tc}$ radio-imaging 1503
- Daniel Derby Asres and Hélène Perreault** A gas-to-solid phase methanolysis method for the analysis of small amounts of oligosaccharides 1512
- Ted Schaefer, Guy M. Bernard, and Frank E. Hruska** An estimate of the spin-spin coupling constant, $^1J(^1\text{H}, ^{13}\text{C})$, in gaseous benzene 1524
- A.B.F. da Silva and M. Trsic** Gaussian- and Slater-type bases for ground and certain low-lying excited states of positive and negative ions of the atoms H through Xe based on the generator coordinate Hartree-Fock method 1526
- Martyn A. Brown, Dennis G. Tuck, and Edward J. Wells** Spectroscopic and crystallographic studies of phosphino adducts of indium(III) iodide 1535
- Khalid Driaf, Robert Granet, Pierre Krausz, Mourad Kaouadji, François Thomasson, Albert José Chulia, Bernard Verneuil, Marenglen Spiro, Jean-Claude Blais, and Gérard Bolbach** Synthesis of glycosylated cationic porphyrins as potential agents in photodynamic therapy 1550
- José Alberto Caram, María Virginia Mirífico, Silvia Lucía Aimone, and Enrique Julio Vasini** 3,4-Disubstituted derivatives of 1,2,5-thiadiazole 1,1-dioxide. Ethanol addition reactions and electroreduction of 3-methyl-4-phenyl and 3,4-dimethyl derivatives in acetonitrile and ethanol solvents 1564
- Katherine N. Robertson, T. Stanley Cameron, and Osvald Knop** Polyhalide anions in crystals. Part 2. I_3^- asymmetry and N—H...I bonding: triiodides of the Me_2NH_2^+ , Ph_2I^+ , tropanium, *N,N,N',N'*- Me_4 -1,2-ethanediammonium, *N,N,N',N'*- Me_4 -1,3-propanediammonium, *N*-*Me*-piperazinium(2+), and *N,N'*- Me_2 -piperazinium(2+) cations, and $\text{Me}_2\text{NH}_2\text{I}$ 1572
- K.C. Majumdar and U. Das** Synthesis of 1-alkoxy-1,2,3,4-tetrahydrocarbazoles by mercury(II) mediated heterocyclization of 2-cyclohex-2'-enyl-*N*-alkylanilines 1592
- M. Soledade C. Pedras** The chemistry of cyclohexenediones produced by the blackleg fungus 1597
- IUPAC recommendations / Recommandations de l'UICPA** iii
- Author Index / Index des auteurs** AI-1

September / Septembre

ARTICLES

- M.A. Biasutti and Juana J. Silber** Interaction between tetracyanoethylene and naphthalene in reverse micelles of AOT in *n*-hexane. The electron-donor properties of AOT 1603
- Rakesh Kumar, Leonard I. Wiebe, and Edward E. Knaus** Synthesis of 5-(1-azidovinyl) and 5-[2-(1-aziriny)] analogs of 2'-deoxyuridine 1609
- Kim Gracie, Dale Turner, and R. Palepu** Thermodynamic properties of micellization of sodium dodecyl sulfate in binary mixtures of ethylene glycol with water 1616
- Ted Schaefer, Guy M. Bernard, Younes Bakkali, and David M. McKinnon** Theoretical and experimental approaches to the effects of solvation on the small internal rotational potential of benzal fluoride 1626
- Kashyapa Ananda Ginige, John Edward Goehl, and Richard Francis Langer** Sulfonyl esters 7. The second and third sequences in the Trithioorthoformate Reaction 1638
- Jean-Luc Pozzo, André Samat, Robert Guglielmetti, Vladimir Lokshin, and Vladimir Minkin** Furo-fused 2*H*-chromenes: synthesis and photochromic properties 1649
- Gerard A. Heal, P. Duane Walker, Michael Ramek, and Paul G. Mezey** Shape-similarity analysis of 20 stable conformations of neutral β -alanine 1660

Jack Passmore, T. Stanley Cameron, Paul D. Boyle, Gabriele Schatte, and Todd Way	The preparation and characterization of $\text{SeCl}_3\text{SbF}_6$, improved syntheses of $\text{MCl}_3(\text{As/Sb})\text{F}_6$ ($\text{M} = \text{S}, \text{Se}$), and the X-ray crystal structure determination of $\text{SeCl}_3\text{AsF}_6$ and a new phase of SBr_3SbF_6	1671
Hélène Perreault and Catherine E. Costello	Differentiation of cerebroside isomers and study of fragmentation by liquid secondary ion mass spectrometry and mass spectrometry/mass spectrometry of selected derivatives	1682
Ying Mu, Warren E. Piers, Donald C. MacQuarrie, and Michael J. Zaworotko	Zirconium complexes of a cyclopentadienylamido ligand with a pendant amine donor via amine and alkane elimination	1696
Yvonne Lear and Tony Durst	Synthesis and biological evaluation of carbon-substituted C-4 derivatives of podophyllotoxin	1704
Georgios Kokkinidis, Achilleas Papoutsis, and Evdokia Coutouli-Argyropoulou	Oxidation pathways of hydroxydopamines and their chloride and bromide salts: an electrochemical study in acidic solutions	1709
Svetlana V. Kudrevich and Johan E. van Lier	Substituted tetra-2,3-pyrazinoporphyrazines. Part II. Bis(tri- <i>n</i> -hexylsiloxy)silicon derivatives	1718
Jocelyn Renaud and J.C. Scaiano	Hydrogen vs. electron transfer mechanisms in the chain decomposition of phenacyl bromides. Use of isotopic labeling as a mechanistic probe	1724
Stephen Hanessian, Hubli Prabhajan, Dongxu Qiu, and Sudhir Nambiar	Synthesis of chemically and functionally diverse scaffolds from pentaerythritol	1731
Stephen Hanessian, Dongxu Qiu, Hubli Prabhajan, Gurijala V. Reddy, and Boliang Lou	Synthesis of clustered D-GalNAc (Tn) and D-Gal β (1 \rightarrow 3)GalNAc (T) antigenic motifs using a pentaerythritol scaffold	1738
F.E. Jorge and A.B.F. da Silva	The generator coordinate Dirac-Fock method applied to beryllium-like atomic species	1748
James P. Kutney, Yong-Huang Chen, and Steven J. Rettig	The chemistry of thujone. XIX. Acid-promoted ring cleavage of thujone-derived cyclopropylcarbinols	1753
COMMUNICATION		
Claude Spino, Laurel Clouston, and David Berg	Novel, air-stable, lanthanide catalysts for the hetero Diels-Alder reaction	1762
Author Index / Index des auteurs		AI-1

October \ Octobre

ARTICLES

H.I. Schiff	1995 Fisher Scientific Award Lecture: Reflections of an atmospheric chemist wondering why he won an analytical chemistry award	1765
Robin A. Cox	The decomposition of aliphatic <i>N</i> -nitro amines in aqueous sulfuric acid. Bisulfate as a nucleophile	1774
Robin A. Cox	The acid-catalyzed decomposition of nitramide	1779
Paul S. Sidhu, Jason Bell, Glenn H. Penner, and Kenneth R. Jeffrey	A deuterium NMR study of guest molecular dynamics in tris(5-acetyl-3-thienyl) methane inclusion compounds	1784
T. Bruce Grindley, Paula J. MacLeod, James A. Pincock, and T. Stanley Cameron	Conformational behaviour of highly hindered ethanes: <i>meso</i> - and racemic-2,2,2',2'-tetramethyl-1,1'-biindanyl	1795
Ted Schaefer, Guy M. Bernard, and Frank E. Hruska	Reflection in the ^1H NMR spectrum of $^{37}\text{Cl}/^{35}\text{Cl}$ isotope effects on the ^{19}F NMR chemical shifts of 1-chloro-2,4-difluorobenzene. An isotope effect over five bonds	1810
J.A. González, J.M. Fernández Martínez, I. García de la Fuente, and J.C. Cobos	DISQUAC characterization of the carbonyl-oxygen interactions in binary liquid organic mixtures containing linear molecules: ketones and a monoether, diether, or triether	1815
A. Irigoras, J.M. Ugalde, X. Lopez, and C. Sarasola	On the dissociation energy of $\text{Ti}(\text{OH}_2)^+$. An MCSCF, CCSD(T), and DFT study	1824
David N. Glew and Norman S. Rath	Aqueous nonelectrolyte solutions. Part XIV. D-ice and D-hydrate freezing points of deuterium oxide-ethylene oxide solutions and the formula of congruent ethylene oxide D-hydrate	1830
Patricia A. Rose, Bo Lei, Angela C. Shaw, M.K. Walker-Simmons, Scott Napper, J. Wilson Quail, and Suzanne R. Abrams	Chiral synthesis of (+)-8'-demethyl abscisic acid	1836
Glenn A. Facey, Terrence J. Connolly, Corinne Bensimon, and Tony Durst	A solid state NMR and X-ray crystallographic investigation of dynamic disorder in solid tetrahydronaphthalene derivatives	1844
Marie Jeanne Quirin, Martine Taran et Bernard Delmond	Fonctionnalisation du δ -pyronène, un nouveau synthon terpénique	1852
Thomas G. Back and Denise L. Baron	Stereoselectivity of directed epoxidations of 22-hydroxy- Δ^{23} -sterol side chains	1857
Tilak P. Wijesekera	5-Perfluoroalkyldipyrromethanes and porphyrins derived therefrom	1868
Arthur E. Martell, Ramunas J. Motekaitis, Dian Chen, Robert D. Hancock, and Derek McManus	Selection of new Fe(III)/Fe(II) chelating agents as catalysts for the oxidation of hydrogen sulfide to sulfur by air	1872
Stephen Hanessian and Sacha Ninkovic	Total synthesis of isodeoxydopodophyllotoxin using the Me_3Sn radical initiated carbocyclization	1880
Christopher Milne and John Milne	Studies on the interaction of selenite and selenium with sulphur donors. Part 5. Thiocyanate	1889

- S. Ahmed and S.K. Saha** Electrochemical study of the reaction between progressively alkylated thiazine leucodyes and Fe(III) on a glassy carbon electrode 1896

COMMUNICATION

- Nick Henry Werstiuk, Chandra Deo Roy, and Jiangong Ma** A study of the vacuum pyrolysis of 11-oxatricyclo[6.2.1.0^{2,7}]undeca-2,9-diene. The HeI ultraviolet photoelectron spectrum of 1,2-cyclohexadiene 1903

Author Index / Index des auteurs

AI-1

November / Novembre

This issue is dedicated to Professor Howard C. Clark
Ce tirage est dédié au Professeur Howard C. Clark

ARTICLES

- Robert H. Morris** 1995 Alcan Award Lecture: New intermediates in the homolytic and heterolytic splitting of dihydrogen 1907
- Mary Anne White** 1996 Noranda Award Lecture: Thermal properties of solids: Étude in three-part anharmonicity 1916
- Waltraud Gasafi-Martin, Gabriele Oberendfellner, and Konrad von Werner** A facile synthesis of metalla-octafluorocyclopentane complexes of ruthenium and nickel 1922
- Richard D. Chambers, Alex J. Roche, and Julian F.S. Vaughan** Direct syntheses of pentakis(trifluoromethyl)cyclopentadienide salts and related systems 1925
- Pietro Berno, Mark Moore, Ravinder Minhas, and Sandro Gambarotta** Monomeric and dimeric V(III) complexes supported by organic amides 1930
- Kenzo Ohkita, Hideo Asano, Hideo Kurosawa, Toshikazu Hirao, Yohko Miyaji, and Isao Ikeda** Observation of buttressing effect and hindered rotation about C(sp²)—C(sp²) single bond in styrenes coordinated to a ruthenium cation, Cp(diphosphine)Ru⁺ 1936
- John M. Stadlbauer, Krishnan Venkateswaran, Hugh A. Gillis, Gerald B. Porter, and David C. Walker** Micelle-induced change of mechanism in the reaction of muonium with acetone 1945
- Changqing Wang, Sun Chau Siu, Germaine Hwang, Christian Bach, Bianca Bley, Matthias Bodenbinder, Helge Willner, and Friedhelm Aubke** Homoleptic carbonyl cations of palladium(I), palladium(II), platinum(II), and gold(I) — simplified synthetic routes to their fluoroantimonate(V) salts 1952
- Bentley J. Palmer and Ross H. Hill** The energetics of the oxidative addition of trisubstituted silanes to photochemically generated (η⁵-C₅R₅)Mn(CO)₂ 1959
- John E. Drake, Robert J. Drake, Layla N. Khasrou, Anil G. Mislankar, Raju Ratnani, and Jincai Yang** Synthesis, spectroscopic and structural studies of *O*-methyl and *O*-isopropyl monothiocarbonate (monoxanthate) derivatives of dimethyl- and diphenyltellurium(IV). Crystal structures of Me₂Te[SCO₂(*i*-Pr)]₂, Ph₂Te[SCO₂(*i*-Pr)]₂, Me₂TeCl[SCO₂Me], and Me₂TeBr[SCO₂(*i*-Pr)] 1968
- Sudhir Achar, Richard J. Puddephatt, and John D. Scott** Organoplatinum(IV) derivatized vinyl monomers and polymers prepared by oxidative addition 1983
- Robert A. Stockland, Jr., Gordon K. Anderson, Nigam P. Rath, Janet Braddock-Wilking, and J. Christopher Ellegood** Synthesis of the complexes [PdCIR(cod)] (R = benzyl, ethyl; cod = 1,5-cyclooctadiene). β-Elimination from [PdClEt(cod)] to give the η¹, η², and η³ isomers of [Pd₂(μ-Cl)₂(C₈H₁₃)₂] 1990
- Andrew R.L. Skauge, Richard D. Shalders, and Thomas W. Swaddle** High-pressure methods as a tool in organometallic syntheses: facilitation of oxidative addition to platinum(II) 1998
- Xiaobo Ou and Alexander F. Janzen** Oxidative fluorination in the Ph₂SO—XeF₂—Cl[−] system and fluorine exchange in the Ph₂S(O)F₂—Ph₂S(O)F⁺ system 2002
- Trevor G. Appleton, Campbell J. D'Alton, John R. Hall, Michael T. Mathieson, and Mark A. Williams** Synthesis of dimethylplatinum(IV) compounds, [(PtMe₂X₂)_n], [(PtMe₂XY)_n], and, in solution, *fac*-[PtMe₂X(H₂O)₃]⁺, where X and Y are anionic ligands 2008
- Anshu Singhal and Vimal K. Jain** Synthesis and characterization of mono- and bi-nuclear palladium(II) and platinum(II) complexes containing acetamidine ligands 2018
- Chaoyang Dai, Graham Stringer, Todd B. Marder, R. Thomas Baker, Andrew J. Scott, William Clegg, and Nicholas C. Norman** Oxidative addition of a B—B bond by an iridium(I) complex: molecular structure of *mer-cis*-[Ir(PMe₃)₃Cl(Bcat)₂] 2026
- Steven J. Trepanier and Suning Wang** Alkylaluminum complexes containing pyridyl amido ligands. Syntheses and characterization of AlMe₂[N(CH₂-2-Py)₂], Al₂Me₃[N(CH₂-2-Py)₂], and Al₂Me₄[2,3,5,6-tetra(2-pyridyl)piperazyl], an unusual carbon-carbon bond coupling product 2032
- Frank E. Smith, Lian Ee Khoo, Ngoh Khang Goh, Rosemary C. Hynes, and George Eng** The synthesis, and molecular and crystal structure of diphenyl(2-oxidonaphthylmethyliminoacetato)tin(IV) 2041
- Edward Piers and Richard D. Tillyer** Pd(0)-catalyzed addition of Me₃SnSnMe₃ to α,β-alkynic aldehydes and ketones. Synthesis of (Z)-β-trimethylstannyl α,β-alkenic aldehydes and ketones. Preparation and synthetic uses of substituted (Z)-4-trimethylstannyl-1,3-butadienes 2048
- Richard P. Schutte, Steven J. Rettig, and Brian R. James** Synthesis, characterization, and reactivity of a ruthenium(II) N,N',N''-tris(2-pyridyl)phosphine complex. X-ray analysis of RuCl₂(PPh₃)(Ppy₃) (py = 2-pyridyl) 2064

- Alaa S. Abd-El-Aziz, Debbie A. Armstrong, Shelly Bernardin, and Harold M. Hutton** Nucleophilic addition to di- and poly-iron arene complex cations 2073
- Zhao Chen, Chet Jablonski, and John Bridson** Evidence for an intramolecular transition metal Arbuzov reaction 2083
- Naveen Chopra, Leslie C. Damude, Philip A.W. Dean, and Jagades J. Vittal** Pyridine-2-selenolate and -2-tellurolate as ligands: a multinuclear (^{77}Se , ^{119}Sn , ^{125}Te) magnetic resonance study of some tin(IV) complexes, and X-ray structural analyses of $\text{Sn}(\text{SPh})_2(2\text{-Se-C}_5\text{H}_4\text{N-N,Se})_2$ and $\text{Sn}(\text{SPh})_{1.85}(2\text{-Se-C}_5\text{H}_4\text{N})_{2.15}$ 2095
- J.R. Stevens and W. Wieczorek** Ionically conducting polyether composites 2106
- István Kovács and Michael C. Baird** Novel (fulvalene)dichromium alkyl and acyl complexes of the types $\text{FvCr}_2(\text{CO})_{6-n}\text{L}_n\text{RR}'$ and $\text{Et}_4\text{N}[\text{FvCr}_2(\text{CO})_{6-n}\text{L}_n\text{R}]$ ($\text{R}, \text{R}' = \text{Me}, \text{CH}_2\text{CN}, \text{COMe}; \text{L} = \text{CO}, \text{PMe}_2\text{Ph}; n = 0, 1, 2$) 2114
- Fernande D. Rochon, André L. Beauchamp, and Corinne Bensimon** Multinuclear NMR spectra of $[\text{Pt}(\text{L})\text{Cl}_3]^-$ ($\text{L} =$ pyridine derivatives) complexes and crystal structure of *trans*- $\text{Pt}(2,6\text{-di}(\text{hydroxymethyl})\text{pyridine})_2\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ 2121
- J. Stephen Hartman, Zheng Yuan, Arnold Fox, and Anh Nguyen** Bis- and tris(amidine)fluoroboron cations and mixed tetrahaloborate anions: NMR studies of mixed boron trihalide adduct redistribution reactions involving amidines as strong nitrogen bases 2131
- Donald R. Arnold, Mary S.W. Chan, and Kimberly A. McManus** Photochemical nucleophile-olefin combination, aromatic substitution (photo-NOCAS) reaction, Part 12. Factors controlling the regiochemistry of the reaction with alcohol as the nucleophile 2143
- William R. Cullen, Steven J. Rettig, and Hongli Zhang** Synthesis of some phosphino- and arsinobenzenechromium tricarbonyl derivatives and metal carbonyl clusters 2167
- Christian Brückner, Veranja Karunaratne, Steven J. Rettig, and David Dolphin** Synthesis of *meso*-phenyl-4,6-dipyrrins, preparation of their Cu(II), Ni(II), and Zn(II) chelates, and structural characterization of bis(*meso*-phenyl-4,6-dipyrrinato)Ni(II) 2182
- Malken Bayrakdarian, Martin J. Davis, Christian Reber, and Davit Zargarian** Absorption spectroscopy of $(\text{Ind})\text{Ni}(\text{PPh}_3)\text{X}$ ($\text{Ind} =$ indenyl, 1-Me-indenyl; $\text{X} = \text{Cl}, \text{Br}, \text{Me}$) and $\text{M}(\text{Ind})_2$ ($\text{M} = \text{Ni}, \text{Ru}; \text{Ind} =$ indenyl) 2194
- Manuel A.S. Aquino, Christopher A. White, Corinne Bensimon, J.E. Greedan, and Robert J. Crutchley** A pentaammineruthenium(III) dimer with the novel bridging ligand 4,4'-dicyanamidobiphenyl dianion 2201
- Neil Burford, Charles L.B. Macdonald, Trenton M. Parks, Gang Wu, Borzena Borecka, Witold Kwiatkowski, and T. Stanley Cameron** Preparation and structure of 2-chloro-1,3-dimethyldiaza-2-arsenane, 1,3-dimethyldiaza-2-arsenanium tetrachlorogallate, and butadiene cycloadducts of diazarsenium cations 2209
- R.R. Martin and Jinjiang Li** Secondary ion mass spectroscopy (SIMS) and kinetics of the catalysis of bisulphite oxidation by aqueous iron 2217
- Mandapati Saraswathi and Jack M. Miller** Study of formation and fragmentation of ionic complexes of polydentate ligands with Al(III) and glycerol by fast atom bombardment mass spectrometry. Part 1: Polydentate ligands 2221
- Jian Z. Xiong, Detong Jiang, Craig E. Dixon, Kim M. Baines, and T.K. Sham** Structure and bonding of organosilicon compounds containing silicon-silicon and silicon-germanium bonds: an X-ray absorption fine structure study 2229
- Yong-Feng Hu, G. Michael Bancroft, Kim H. Tan, John S. Tse, and Dong-Sheng Yang** Variable-energy photoelectron spectroscopy of $\text{CpM}(\text{CO})_3$ ($\text{M} = \text{Mn}, \text{Re}$) and $\text{CpFe}(\text{CO})_2\text{I}$ 2240
- George Tsaprailis and Ann M. English** Redox activity of tryptophan residues in recombinant cytochrome c peroxidase and its W51F and W191F mutants 2250
- James A. Dunn, Hari K. Gupta, Alex D. Bain, and Michael J. McGlinchey** The metal-mediated conversion of octachlorocycloheptatriene into dodecachloroheptafulvalene: a synthetic, structural, and EHMO study 2258
- Pierre D. Harvey, Réjean Provencher, Jonathan Gagnon, Tianle Zhang, Daniel Fortin, Karine Hierro, Marc Drouin, and Steve M. Socol** Photoinduced oxidative degradation of unsaturated $\text{M}_3(\text{dppm})_3\text{CO}^{2+}$ clusters ($\text{M} = \text{Pd}, \text{Pt}$) by chlorocarbons and chloride ion 2268
- Pierre D. Harvey, Jonathan Gagnon, Réjean Provencher, Bing Xu, and Timothy M. Swager** Tungsten and molybdenum oxo complexes of tetrakis(phenyldiazanyl)calix[4]arene substituted derivatives: EHMO calculations, spectroscopic characterization, and perturbations of the photophysical properties by neutral guest molecules 2279
- Darren S.A. George, Robert McDonald, and Martin Cowie** Parallel vs. perpendicular alkyne coordination in binuclear complexes. The first examples of reactivity differences in isomers differing in their alkyne coordination modes 2289
- Shuquan Song and Elmer C. Alyea** Steric effects of bulky phosphines on ^{95}Mo NMR shieldings 2304
- A.C. Chen, S.G. Sun, D.F. Yang, B. Pettinger, and J. Lipkowski** In situ FTIR studies of 4-cyanopyridine adsorption at the Au(111) electrode 2321
- Sean R. Klopfenstein, Constanze Kluwe, Kristin Kirschbaum, and Julian A. Davies** The reactions of $[\text{Pd}_2\text{Cl}_2(\mu\text{-PP})_2]$ ($\text{PP} = \text{dppm}, \text{dmpm}$) with $\text{Et}_2\text{NC}\equiv\text{CNEt}_2$ in methylene chloride solution: X-ray crystal structures of $[\text{Pd}_2\text{Cl}_2(\mu\text{-CH}_2)(\mu\text{-dppm})_2]$ and hexakis(diethylamino)benzene, $\text{C}_6(\text{NEt}_2)_6$ 2331
- C. Robert Lucas and Shuang Liu** Thiophenophane metal complexes. IV. Effects from ligand changes outside the coordination sphere 2340
- Peter Blenkiron, John F. Corrigan, Didier Pilette, Nicholas J. Taylor, and Arthur J. Carty** Polycarbon ligands: synthesis and characterization of the phosphinodienes $\text{Ph}_2\text{PC}\equiv\text{C-C}\equiv\text{CR}$ ($\text{R} = \text{Bu}^t, \text{Ph}, \text{SiMe}_3$), the $\mu\text{-}\eta^1, \eta^2_{\alpha\beta}$ -butadiynyl complexes $\text{Ru}_2(\text{CO})_6(\mu\text{-PPh}_2)(\mu\text{-}\eta^1, \eta^2_{\alpha\beta}\text{-C}\equiv\text{C-C}\equiv\text{CR})$, and the molecular structure of a cobalt carbonyl derivative $\text{Ru}_2(\text{CO})_6(\mu\text{-PPh}_2)(\mu\text{-}\eta^1, \eta^2_{\alpha\beta}\text{-}\mu\text{-}\eta^2, \eta^2_{\gamma\delta}\text{-C}\equiv\text{C-C}\equiv\text{CBu}^t)\text{Co}_2(\text{CO})_6$ 2349

Nicole Sandblom, Tom Ziegler, and Tristram Chivers A density functional study of the bonding in tertiary phosphine chalcogenides and related molecules	2263
Klaus Eichele, Roderick E. Wasylishen, Robert W. Schurko, Neil Burford, and W. Alex Whitla An unusually large value of $^1J(^{31}\text{P}, ^{31}\text{P})$ for a solid triphenylphosphine phosphadiazonium cationic complex: determination of the sign of J from 2D spin-echo experiments	2372
Jin Li, Kattesh V. Katti, A. Alan Pinkerton, Herbert Nar, and Ronald G. Cavell Synthesis and characterization of phosphinimine-substituted trifluoro- or trichloro- <i>p</i> -benzoquinones and their cationic Rh(I) complexes. The crystal and molecular structure of 3,5,6-trichloro-2-(triphenylphosphinimino)- <i>p</i> -benzoquinone	2378
Theodore A. Budzichowski, Malcolm H. Chisholm, and William E. Streib $\text{Mo}_2(\text{OCH}_2\text{Bu})_6(\text{Cp})\text{Na}(\text{DME})$. Preparation, structure, and solution behavior	2386
COMMUNICATION	
B. Bley, M. Bodenbinder, G. Balzer, H. Willner, G. Hägele, F. Mistry, and F. Aubke Synthesis and spectroscopic characterization of bis(trifluorophosphinyl)-gold(I) undecafluorodiantimonate(V) $[\text{Au}(\text{PF}_3)_2][\text{Sb}_2\text{F}_{11}]$	2392
Author Index / Index des auteurs	AI-1

December / Décembre

ARTICLES

Ronald Kluger, Xianfeng Li, and Richard W. Loo 1996 Bader Award Lecture: Aminoacyl ethyl phosphates. Biomimetically activated amino acids	2395
Elizabeth A. Lund, Isaac A. Kennedy, and Alex G. Fallis Dihydrofurans from α -diazoketones due to facile ring opening – cyclization of donor–acceptor cyclopropane intermediates	2401
Long Mao, Steven J. Rettig, Robert C. Thompson, James Trotter, and Shihua Xia Extended chain 2,3-pyrazinedicarboxylate complexes of manganese(II) and cadmium(II); synthesis and structure and magnetic properties	2413
Luc Ruest and Marco Dodier Ryanoids and related compounds. Identification of five new ryanoids from the plant <i>Ryania speciosa</i> Vahl. Formal total syntheses of 3-deoxyryanodol (cinnzeylanol), 10- <i>O</i> -acetyl-3-deoxyryanodol (cinnzeylanine), 2-deoxyryanodol, 2-deoxy-2-epiryranodol, 2,3-dideoxy-2,3-dihydroryanodol, 2-deoxy-3-epiryranodol, and 2-deoxy-3-epiryranodine	2424
Sibel Mill and Claude Hootelé A revised structure for the piperidine alkaloid andrachamine	2434
Mark Plehiers and Claude Hootelé Synthesis of β -hydroxypiperidine alkaloids by anodic oxidation of carbamates and hydroboration	2444
Teresa María Borges Miquel, Mercedes Lemus Sánchez, Josefa Castro Macías, and Jesús César Rodríguez Placeres Study of the coordinated system Pb(II) – neutral valine – valinate ion	2454
Roy Carl Boerschke, Elizabeth Ann Gallie, Nelson Belzile, Richard Neville Gedy, and James Robert Morris Quantitative elemental and structural analysis of dissolved organic carbon fractions from lakes near Sudbury, Ontario	2460
Aurelio San-Martín, Elías Quezada, Pilar Soto, Yolanda Palacios, and Juana Roviroso Labdane diterpenes from the marine pulmonate gastropod <i>Trimusculus peruvianus</i>	2471
Jose M. Elorza and Jesus M. Ugalde Theoretical study of the PSi_2 radical	2476
J.R. Keffe and A.J. Kresge Solvent and substrate isotope effects on the enolization and carbon-acid ionization of isobutyrophenone	2481
Takashi Tokoroyama and Hisashi Kusaka Folding strain stereocontrol in cyclohexane ring formation by means of an intramolecular ester enolate alkylation reaction	2487
John Washington and Clifford P. Kubiak Reflectance infrared and UV–visible spectroelectrochemical studies on a series of $[\text{Ni}_3(\mu_3\text{-L})(\mu_3\text{-I})(\mu_2\text{-dppm})_3][\text{PF}_6]$ ($\text{L} = \text{CO}$; CNR , $\text{R} = \text{alkyl}$, aryl ; $\text{dppm} = \text{Ph}_2\text{PCH}_2\text{PPh}_2$) clusters	2503
Jamila Jennane, Tanya Boutros, and Richard Giasson Photolithography of self-assembled monolayers: optimization of protecting groups by an electroanalytical method	2509
Earl MacKnight and Robert A. McClelland A photochemical retro-Friedel–Crafts alkylation. Rapid rearrangement of cyclohexadienyl cations	2518
T.V. Pham and K.C. Westaway Solvent effects on nucleophilic substitution reactions. III. The effect of adding an inert salt on the structure of the $\text{S}_{\text{N}}2$ transition state	2528
Bruce J. Balcom and Nils O. Petersen Nitrobenzoxadiazole-labelled polyisoprenoid alcohols	2531
COMMUNICATION	
N.H. Werstiuk, J. Ma, C.D. Roy, A.J. Kresge, and E.A. Jefferson A study of the vacuum pyrolysis of 4-diazoisothiochroman-3-one with HeI ultraviolet photoelectron spectroscopy	2536
ADDITIONS AND CORRECTIONS / AJOUTS ET CORRECTIONS	
Stephen Hanessian, Hubli Prabhanjan, Dongxu Qiu, and Sudhir Nambiar Synthesis of chemically and functionally diverse scaffolds from pentaerythritol	2540
Author Index / Index des auteurs	AI-1